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Atomic-scale investigation of deformation mechanisms in Mg alloys

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ABSTRACT

Mg alloys have excellent strength to weight ratio but their use is limited by their poor room temperature formability. The underlying hexagonal closed pack structure results in a highly anisotropic deformation; basal deformation is easily activated, whereas high stresses are required to accommodate the deformation along <c> axis. We study the atomic-scale mechanisms of Mg nonbasal deformation modes that involve <c + a> slip and twinning. Our study includes two aspects: accurate modeling of defect structures and interactions with solutes and investigation of solute strengthening. The core structures of <c+a> edge and screw dislocations in Mg are computed using density functional theory (DFT). Both types dissociate into two ½<c+a> partials on the second-order pyramidal planes. We show that earlier <c+a> core structures based on embedded-atom method are artifacts of the interatomic potentials and are not accurate. The DFT core structures are used for further investigation of solute effects. In addition, solute strengthening of twin dislocation motion along an existing twin boundary in Mg-X (X = Al, Zn) is investigated using a new Labusch-type weak pinning model. New features emerge in the application of the model because of the very small Burgers vector of the twin dislocation. The strengthening is not large, e.g., a strength of ≈10 MPa is predicted for the AZ31 alloy, but the analysis does predict larger strengthening of twinning compared with basal slip at room temperature and various concentrations. The predictions are compared with existing experimental data and are shown to agree well with the experiments. The methods discussed here, can be applied to a wide range of defect calculations with chemistry change, guiding towards a well-informed design of materials on an accurate foundation.